

LA-UR-21-24248

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Title: The iRage Cookbook

Author(s): Mercer-Smith, James Alastair

Intended for: In-line help package

Issued: 2021-05-03



The iRage Cookbook

Jas. Mercer-Smith, XTD-PRI

Abstract

iRage is a family of Zsh and Python 3 scripts designed to accelerate the process of submitting calculations for the novice xRage user.

iRage reduces the time to write a new input deck and submit an xRage problem to the production queue to about 15 minutes, assuming the user has defined the initial geometry using a program like Osito or linked to problem geometries generated by codes such as Abaqus, Flag, or Pagosa.

iRage runs on Linux and Mac systems.



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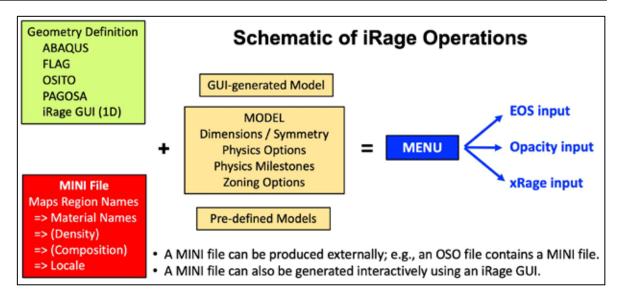
The iRage command line; e.g., "iRage new=myjob now"



- If the iRage user sources the EAP .cshrc file, then the command "iRage" is already aliased; otherwise, the user can set an alias:
- iRage 'zsh /usr/projects/eap/tools/iRAGE/iRage.zsh'
- While iRage is a Zsh script that calls Python 3, it was designed to be run from the default Cshell.
- The iRage command line has two arguments. The first argument triggers iRage options. The second argument defines how a job is submitted to the production queue. For example for problem arbitrarily named "myjob", the command line "iRage new=myjob now" will:
 - Guide the user through GUIs that offer a variety of physics options. Generate EOS and Opacity tables. Produce the rage.input deck. Create a log file. Store the files in the /scratch/moniker/myjob directory, and submit an xRage job to the production queue.
- The iRage toolkit has other useful capabilities, including: analytic contour generation, material properties lookup, and the calculation of normalized isotopic mixtures.
- Command line options are described in the help package called by the command "iRage help".

iRage assembles input decks from MODEL and MINI files.

- A MODEL is a set of physics model options and milestones that specify when physics approximations should be turned on or off.
- A MODEL can be pre-defined or iRage can generate a MODEL interactively using a GUI.



- A MINI file contains: (1) the path to the geometry file, (2) the dimensions of the hydrodynamic mesh, and (3) a mapping from "Region" names (aka, parts) to "Material" names.
 - The Region <=> Material mapping, which includes the options for non-default densities and compositions, can be generated externally by a tool like Osito or internally with an iRage GUI.
- iRage combines a MODEL with a MINI file to produce a MENU file, which has all of the information necessary to generate an xRage input deck.

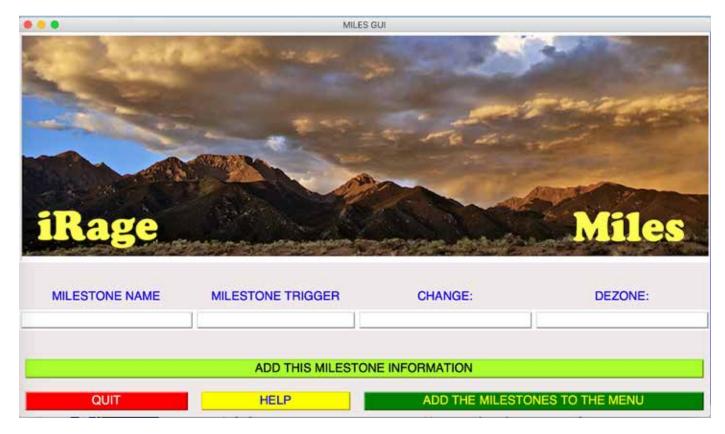


iRage has GUIs that can create new xRage input decks.



- When generating a new problem, iRage calls the "New" GUI which has dropdown menus to define physics model options, the problem geometry, and triggers for additional GUIs that define the mesh, the region-material mapping, and any restart milestones.
- iRage can extract information about the mesh dimensions and the the region <=> material mapping from a MINI file or an OSO file if either exists. This may circumvent the need to call the "Mesh" GUI and/or or the "Map" GUI.
- Specifying the geometry and a pre-defined model provides sufficient information to submit a new xRage simulation from the iRage command line; e.g., 'iRage new.mod=myjob.oso new'.

The xRage restart block is a powerful tool. The iRage "Miles" GUI can set restart blocks at specified milestones.



• The milestone name is arbitrary. The milestone trigger defines the xRage restart block; e.g., "time .gt. 47". The change command inserts an xRage command or triggers an iRage physics model option; e.g., "_radiation on". The dezone command specifies a locale and a power of two dezoning factor; e.g., "DET 4".



The iRage "Map" GUI defines the regions ⇔ materials map interactively. This mapping produces a MINI file.



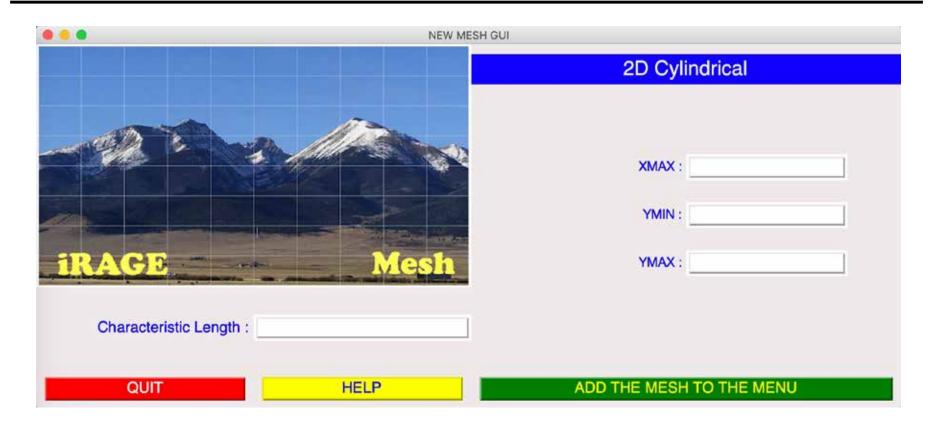
- Each Region
 Anaterial mapping permits the user to override the default density, and material composition.
- The completed map is a MINI file. iRage then generates a MENU file, as well as the "rage.input" deck whether or not the user has specified a geometry file.

The iRage "1D Map" GUI builds pie diagrams interactively.



- In 1D, the region names are defined by the outer radius of each shell. The user has a dropdown menu to select either the mass or the outer radius for each shell.
- The pie diagram with both radii and masses is stored in the 1D MINI file.

The iRage "Mesh" GUI defines the hydro mesh dimensions.



- The "Dimensions / Symmetry" option on the "New" GUI page defaults to "2D Cylindrical".
- iRage calculates the optimal Level 1 mesh size automatically.

The iRage "Dets" GUI sets HE detonation point locations.



- The iRage "Dets" GUI page is only called if the user selected a high explosive model on the "New" GUI page.
- iRage has the option to add as many detonation points as the user may desire.

A MINI file identifies the geometry and region ⇔ material map; the "Mini" GUI can add the physics MODEL options.

```
******
                                   tmp37.mini
                                                            ***********
*// project:
               tmp37
*// model:
                                        ! Pre-defined model for testing
                ias
*// geofile:
                                        ! oso (OSITO-generated geometry file)
               test.oso
BEGIN REGINFO
                                3 0.025 1.0e6 0 1 LOC // !=Default copper, @=Part 123,
reg1
               copper
202
               salt
                                3 0.025 1.0e6 0 1 LOC // !=Not iodized, %m na 0.49 cl 0.49 %
                                3 0.025 1.0e6 0 1 HEX // !=Default PBX-9501 charge B, @=Part 789B,
reg_charge:B
               pbx9501:B
                                3 0.025 1.0e6 0 1 LZ2 // rho=.52, %m h 0.52 c 0.48 %
reg52
               polystyrene:52
BEGIN BBOX
             0.0 127.0 -127.0
                                127.0
                                                       0.0 // xmin, xmax, ymin, ymax, zmin, zmax, clength
                                         0.0
                                                0.0
```



- The information in a MINI file, combined with physics options and a geometry file, is both necessary and sufficient to uniquely define the input deck for an xRage simulation.
- The format of a '.mini" file is the same as the REGINFO block of an OSO file.
- "iRage mini=myjob" can use a MINI file to link Abaqus, Flag, or Pagosa calculations to xRage.
- "iRage mini.new=myjob" calls a GUI to allow for the interactive selection of physics options, while "iRage mini.mod=myjob" invokes the pre-defined options of the "mod" model.

Pre-defined models provide the iRage user with shortcuts; e.g., "iRage new.mod=myjob.oso now".

```
iRmod_jas.txt
*// model:
                  jas
                                         ! A model for testing purposes
*// quality:
                                         ! Default physics options and zoning
                  good
 // geometry:
                  2D Cylindrical
                                         ! Dimensions / Symmetry
 // hydrobc:
                  Mirror
                                         ! Hydro Boundary: Mirror, Vacuum
 // radbc:
                  Vacuum
                                         ! Rad Boundary: Mirror, Vacuum, T(time)
 *// units:
                                         ! Mesh zoning units
                  micron
 '// hydro:
                  ip6
                                         ! Options: ip0, ip1, ip2, ip4, ip6, vof
                                         ! Options: off, ep, jc, kos, ptw, ptw1, sg
 // strength:
 // explosives:
                  cg_mie.jwl
                                         ! Options: off, (cg,ff,hi,so,sp).(hom,jwl,mie
 // conduction:
                  spitzer
                                         ! Options: off, sesame, spitzer
 // radiation:
                                         ! Options: off, gd, mgd
                  opc20_lte
 // opacity:
                                         ! Options: off, opc(20,25,30,58)_(lte,nlte)
*// plasma:
                  3t
                                         ! Options: off, 2t, 3t
 *// lasers:
                  off
                                         ! Options: off, lle, nif
                  off
                                          ! Options: off, bhr2, bhr3, modal
*// tstop:
                  1.0e-4
                                         ! Forced stop time, tmax = 1.0e-4.
&// milestone:
                  time .ge. 0.0
                                         ! Begin simulation @ start
&// change:
                  par = 0.0
                                         ! Set parameter par @ start
&// change:
                  par2 = 0.0
                                         ! Set parameter par2 @ start
&// change:
                  _radiation on
                                         ! Turn on radiation @ start
&// milestone:
                  time .qt. 1
                                         ! Trigger restart milestone @ mile1
&// change:
                  par = 1.1
                                         ! Change parameter par @ mile1
&// change:
                  _conduction
                                         ! Turn on conduction @ mile1
&// change:
                  _radiation
                                         ! Turn on specified radiation model @ mile1
&// change:
                  _plasma
                                         ! Turn on 2T @ mile1
&// dezone:
                  det 2
                                          ! Dezone: locale factor @ mile1
&// milestone:
                  time .gt. 2
                                         ! Trigger restart milestone @ mile2
&// change:
                  par = 2.2
                                         ! Insert: line @ mile2
&// dezone:
                  det 4
                                         ! Dezone: locale factor @ mile2
&// dezone:
                                          ! Dezone: locale factor @ mile2
                  hex 2
```

- iRage has several pre-defined model options available.
 - The MODEL specifies the physics approximations that will be used in the xRage input deck. The physics models are indicated by *// cards.
 - The MODEL also specifies the actions that xRage will take at each of the milestones. These are indicated by &// cards.
- The iRage user also has the option to customize a MODEL named "mod" that can be called from local file space.
- The cited shortcut submits an OSO file directly to production with no further user intervention.



The MENU file may be a handy shortcut for the iRage user.

- iRage automatically generates a ".menu" file which combines the physics options specified by the MODEL with the ".mini" file produced by the the "Map" GUI.
- It may be convenient for a user to change physics options, parameters, zoning, etc. in the MENU file; and then run iRage again. For example,

iRage menu=myjob run

uses the information in the "myjob.menu" file to produce a new "rage.input" deck without having to call any of the GUIs. The "run" flag indicates that the job is submitted to the production queue under the assumption that the EOS and Opacity files already exist.

 Note that in the example the geometry file was not defined. iRage will build the input file; but xRage would crash.

```
// project:
                 tmp1
                  210322x
   pname:
  / xraae:
// cpuhrs:
                  36-8
// propath:
                 /Users/jasm-s/scratch/jasm-s/tmp1
 // geofile:
                 /Users/jasm-s/scratch/jasm-s/tm31/UNKNOWN
   eosfile:
                 /Users/jasm-s/scratch/jasm-s/tmp1/tmp1.
  opcfile:
                 /Users/jasm-s/scratch/jasm-s/tmp1/tmp1.opc20
// model:
                 jas
                                         ! A model for testing purposes
 // quality:
                 good
                                         ! Default physics options and zoning
                 2D Cylindrical
// geometry:
                                         ! Dimensions / Symmetry
                                          ! Hydro Boundary: Mirror, Vacuum
 / hydrobc:
                 Mirror
 / radbc:
                 Vacuum
                                          ! Rad Boundary: Mirror, Vacuum, T(time)
// units:
                  micron
                                          ! Mesh zoning units
*// hvdro:
                 ip6
                                         ! Options: ip0, ip1, ip2, ip4, ip6, vof
                                         ! Options: off, ep, jc, kos, ptw, ptw1, sg
 // strength:
  / explosives:
                 cg_mie.jwl
                                         ! Options: off, (cg,ff,hi,so,sp).(hom,jwl,mie
                 spitzer
                                          ! Options: off, sesame, spitzer
                                          ! Options: off, gd, mgd
                 opc20_lte
                                          ! Options: off, opc(20,25,30,58)_(lte,nlte)
                                          ! Options: off, 2t, 3t
  plasma:
 / lasers:
                 off
                                         ! Options: off, lle, nif
*// mix:
                 off
                                          ! Options: off, bhr2, bhr3, modal
*// tstop:
                                         ! Forced stop time, tmax = 1.0e-4.
                 1.0e-4
// level1:
                 0.8192
                                          ! Level 1 mesh size (cm)
// hydromesh:
                 0.0 130.0 -130.0 130.0
                                                             0.0 ! xmin xmax ymin ymax
// detpoint:
                                                                   xdet vdet zdet Rdet
*// detpoint:
                                                                 ! xdet ydet zdet Rdet
   xensight:
                   grd mat rho tev prs vel
                   grd mat rho tev prs vel
                 rho rev tev prs vel
*// tracers:
```



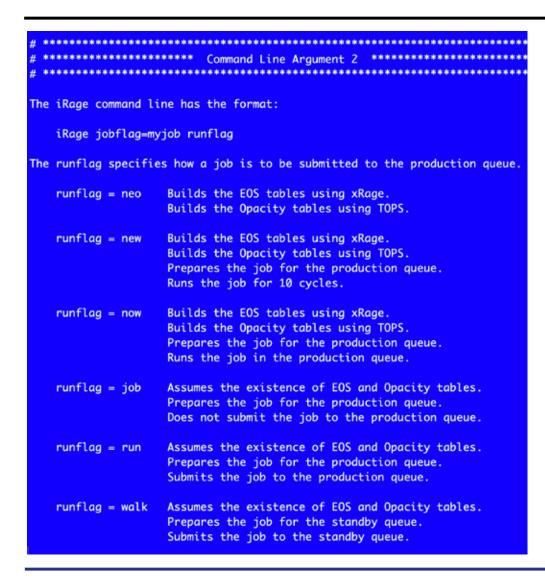
iRage produces well-documented xRage input decks.

```
! ** Hydro Method Options
dohydro = .true.
                                         ! Turn on hydrodynamics.
hydro_version = 2
                                         ! Current Rage hydro version
fvolpct = 0.01
                                         ! Mesh refinement on material gradient
 ho_floor = 1.0e-6
                                         ! Minimum density in a cell
                                         ! Gittings-van Leer limiter
 numrho = 6
                                         ! 0-No IP, 1-IP, 3-VOF
interface_option = 1
shock_detector = 2
                                         ! 1=IP off, 2=IP on
numreg = 16
                                         ! Number of regions
nummat = 14
                                         ! Number of materials
ramp_num = 5
                                         ! Number of ramped materials
ramp_reverse(1) = 5 * .false.
                                         ! All ramps are irreversible
cq_number = 2
                                         ! Number of Cerro Grande materials
cq_size = 0.0128
                                         ! Cerro Grande cell size
cq_dtpct = 0.4
                                         ! Cerro Grande time step change
cq_p_time = 0.13e-6
                                         ! Cerro Grand p-time change
 ** Material 1: BAKair
matident(1) = 'BAKair'
                                         ! Nickname: Rho=0.0013, Abar=14.8028
matdef(1, 1) = 5030
                                         ! EOS; Rhoeos=0.0013, Abareos=14.5481
matdef(25, 1) = 0.982794
                                         ! Scalina Ratio, SR = Abareos/Abar
matdef(61, 1) = 65030
                                         ! Ipcress opacity table.
 ** Map Region 1 (Background) <=> Material 1 (BAKair)
mnamereg(1) = 'Background'
                                         ! Background air
matreg(1) = 1
                                         ! Region 1 <=> Material 1
rhoreg(1) = 0.0013
                                         ! Initial density (q/cc)
tevreg(1) = 0.025
                                         ! STP temperature (eV)
 Material 1 (BAKair) Initial Zoning
sizebnd(1) = 1.6384
                                         ! Level 1 zoning for material boundary
                                         ! Level 1 zoning for material interior
sizemat(1) = 1.6384
```

- iRage produces "rage.input" decks which have comments on every line.
- Well-documented input decks can serve as text books on the numerical and physical approximations available to a code.

```
. . . . . . . . . . . . . . . . . . .
 ******* Radiation Physics ********
                                         ! Turn on radiation physics.
 ** Radiation Boundary Conditions: 2D Cylindrical Symmetry
                                          ! Reflective boundary left (xmin)
tevcl = 0.0
tevcr = 0.01
                                         ! Vacuum boundary right (xmax)
tevcb = 0.01
                                         ! Vacuum boundary below (ymin)
tevca = 0.01
                                         ! Vacuum boundary above (ymax)
 ** Planck vs Rosseland Mean Opacities
ipcress_do_planck_ff = .false.
                                          ! Max(Rosseland absorption, Planck FF)
ipcress_use_pgray_mat(1) = 17 * .true.
                                         ! T - Planck FF; F - Rosseland
do_rad_noneq_correct = .false.
                                          ! Forego accuracy for stability
kapmin = 1.0e-20
                                         ! Minimum absorption coefficient (def 1e-6)
 ** Diffusion Approximation
fluxlim = .true.
                                          ! Levermore flux-limited diffusion
 taxph4loop = 1
                                          ! Iterations to converge matter-rad coupling
                                          ! Default solver 1D/2D
solver_option = 50
 ** Insert at milestone start
par = 0.0
                                         ! Insert: line @ start
```

The iRage command line has a "runflag" that simplifies the submission of jobs to the production queue.

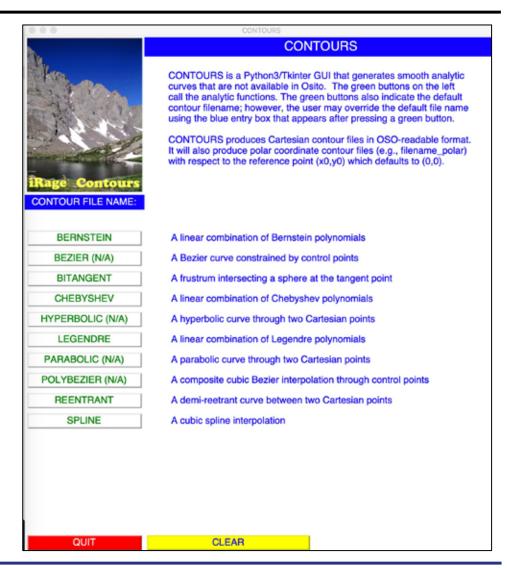


- Submitting jobs to the production queue can be a mysterious process for the novice xRage user.
 - First the user runs xRage to create EOS tables. Then the user runs TOPS to produce Opacity tables.
 - Then the user builds a fine named "run_job.csh" in order to take advantage of the EAP production scripts.
 - Then the user moves the xRage input file, the geometry file, the EOS file, the Opacity file to scratch space, and finally submits the job to the production queue.
- iRage takes care of all of this with a single flag that provides the user several options for submitting jobs.



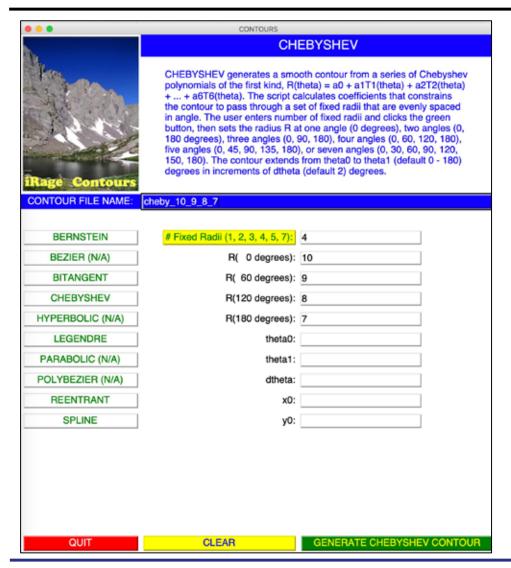
Other iRage tools: Contours ("iRage con")

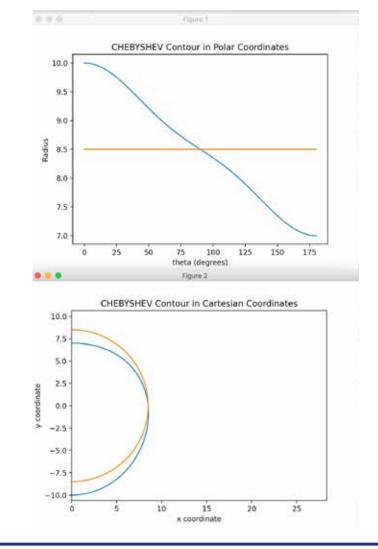
- iRage Contours provides several analytic contours that supplement the analytic functions that are available in Osito. The command "iRage contours" (or "iRage con") calls a selection of GUIs which generate: Bernstein, Bezier, bitangent, Chebyshev, hyperbolic, Legendre, parabolic, polybezier, reentrant, and spline contours.
- The GUIs generate contours in both Cartesian and polar coordinates. The Cartesian coordinates are written in the OSO format that can be read directly by Osito and xRage.





Example of the CHEBYSHEV contour option.





Other iRage tools: Material Lookups (e.g., "iRage steel")

```
Zsh ~/JAS> iRage sst
                                                                            Zsh ~/JAS> iRage 4272
iRage version 210202 @ 16:46:56
                                                                             iRage version 210202 @ 16:47:30
Material Name : sst
                                                                            Material Name : sst
  Sesame EOS : 4272
                                        Sesame OPC : 00000
                                                                              Sesame EOS : 4272
                                                                                                                     Sesame OPC : 00000
  Sesame Abar : 55.3650
                                        Ipcress OPC: 64272
                                                                              Sesame Abar : 55.3650
                                                                                                                     Ipcress OPC: 64272
  Sesame Zbar : 25.8020
                                        Conduction : 24279
                                                                              Sesame Zbar : 25.8020
                                                                                                                     Conduction : 24279
  Sesame Rho0 : 7.8960
                                                                              Sesame Rho0 : 7.8960
                                        Abar : 55.3621
  Normalized Composition
                                                                               Normalized Composition
                                                                                                                     Abar : 55.3621
                                        Zbar: 25.8030
Element % Moles % Weight
                                                                            Element % Moles % Weight
                                                                                                                     Zbar: 25.8030
 cr
        0.202300
                   0.190000
                                                                                               0.190000
                                                                                     0.202300
 fe
        0.693900
                   0.700000
                                                                             fe
                                                                                     0.693900
                                                                                               0.700000
        0.103800 0.110000
 nί
                                                                                     0.103800 0.110000
Elastic-Plastic Strength Model: sst
                                                                            Elastic-Plastic Strength Model: 4272
  matdef 5: -3.0e10
                                        Fail pressure (erg/cc)
                                                                                      5 : -3.0e10
                                                                                                                     Fail pressure (erg/cc)
                                        Shear modulus
  matdef 7 : 7.70e11
                                                                                      7 : 7.70e11
                                                                                                                     Shear modulus
  matdef 12: 3.40e9
                                        Yield stress
                                                                              matdef 12: 3.40e9
                                                                                                                     Yield stress
  matdef 13 : 1.0e10
                                        Elastic pressure
                                                                              matdef 13 : 1.0e10
                                                                                                                     Elastic pressure
Steinberg-Guinan Flow-Stress Model: sst
                                                                            Steinberg-Guinan Flow-Stress Model: 4272
  matdef 101 : 7.90
                                        SG reference density (a/cc)
                                                                              matdef 101 : 7.90
                                                                                                                     SG reference density (q/cc)
  matdef 102 : 7.70e11
                                        GO. shear modulus (era/cc)
                                                                              matdef 102 : 7.70e11
                                                                                                                     GO, shear modulus (erg/cc)
  matdef 103 : 3.4e9
                                        Y0, yield strength (erg/cc)
                                                                              matdef 103 : 3.4e9
                                                                                                                     Y0, yield strength (erg/cc)
  matdef 104 : 2.26e-12
                                        A. P-dep shear modulus (cc/era)
                                                                               matdef 104 : 2.26e-12
                                                                                                                     A, P-dep shear modulus (cc/erg)
  matdef 105 : 5.280
                                        B, T-dep shear modulus (1/eV)
                                                                               matdef 105 : 5.280
                                                                                                                     B. T-dep shear modulus (1/eV)
  matdef 106 : 43.0
                                        beta work hardening parameter
                                                                               matdef 106 : 43.0
                                                                                                                     beta work hardening parameter
  matdef 107 : 0.35
                                        n work hardening parameter
                                                                               matdef 107 : 0.35
                                                                                                                     n work hardening parameter
  matdef 108 : 0.00
                                        ep0, initial plastic strain
                                                                               matdef 108 : 0.00
                                                                                                                     ep0, initial plastic strain
  matdef 109 : 25.0e9
                                        Ymax, Max yield strength (erg/cc)
                                                                               matdef 109 : 25.0e9
                                                                                                                     Ymax, Max yield strength (erg/cc)
  matdef 110 : 1.93
                                        Initial Gruenisen gamma
                                                                               matdef 110 : 1.93
                                                                                                                     Initial Gruenisen gamma
                                        V-dep gamma coefficient
  matdef 111 : 1.4
                                                                              matdef 111 : 1.4
                                                                                                                     V-dep gamma coefficient
                                        Tmelt, melt temp (eV)
  matdef 112 : 0.205
                                                                               matdef 112 : 0.205
                                                                                                                     Tmelt, melt temp (eV)
iRage Finis @ 16:46:56
                                                                             iRage Finis @ 16:47:30
```

iRage performs material lookups and reverse (EOS) lookups; e.g., "iRage sst" or "iRage 4272"



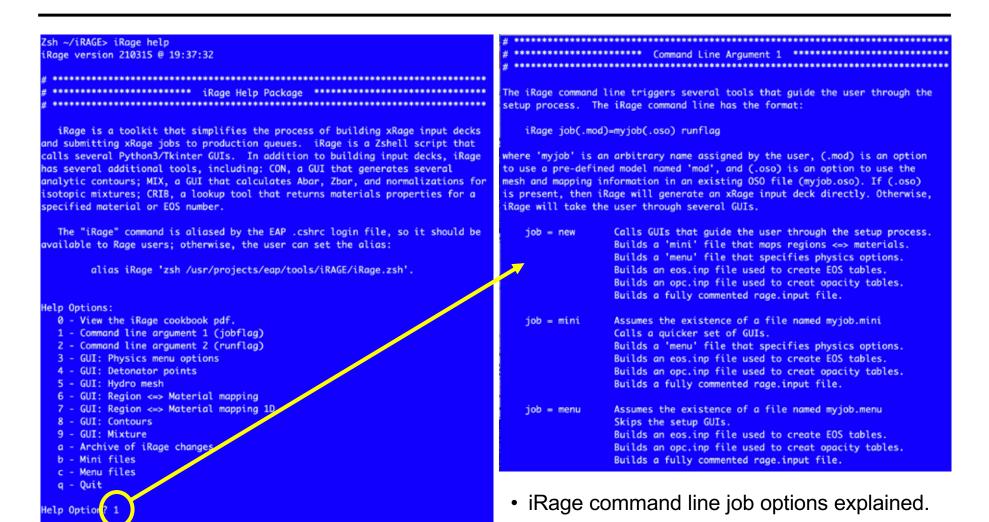
Other iRage tools: Mixtures ("iRage mix")



• "iRage mix" calls a GUI which calculates Abar, Zbar, and normalized isotopic mixtures by molar number and weight. Note that the GUI accepts input in either moles or weight for each of the isotopes in the mixture with the default being moles.



"iRage help" triggers the inline help package.



• iRage has help packages that can be called either from the command line or from the GUIs.



Some final comments about iRage.

- iRage is a toolkit that produces well-documented xRage input decks
- iRage can automatically submit xRage simulations to the production queue.
- iRage is an example of how the setup process can be simplified through the use of GUIs.
- iRage was designed to focus the attention of novice xRage users on selecting appropriate physics approximations rather than worrying about input deck syntax.

